possibilities for interactive consultation.
Keywords: physical properties of crystals, tensor properties, phase transitions

OCM07.27.5
Acta Cryst. (2005). A**61**, C132
International Tables for Crystallography, Volume A1
Ulrich Müller[a], Hans Wondratschek[b], [a]*Fachbereich Chemie, Philipps-Universität, D-35032 Marburg, Germany.* [b]*Institut für Kristallographie, Universität, D-76128 Karlsruhe, Germany.* E-mail: mueller@chemie.uni-marburg.de

The list of the maximal subgroups of the space groups in Volume *A* is incomplete. Volume *A*1 [1] now contains the complete data. Its Part 1 deals with group-theoretical aspects of space groups, group–subgroup relations and the underlying mathematical background. Part 2 contains complete listings of all maximal subgroups for each space group, including their general positions or their generators, their conjugacy relations and transformations to conventional settings. Part 3 lists the relations between the Wyckoff positions for every maximal subgroup of every space group, including the cell transformations and coordinate transformations. In both parts the infinitely many isomorphic subgroups have been included in a parametrized form.

The importance of listing all subgroups individually, not just their types, can be seen in the relations of the AlB_2 structure (*P*6/*mmm*) with those of ZrBeSi and $CaIn_2$ which crystallize in two *different* subgroups $P6_3/mmc$. The occupied atomic positions of AlB_2 split in different ways to the positions of the two subgroups [2].

The index of symmetry reduction to a maximal isomorphic subgroup may adopt an infinity of values, e.g. p = prime = $6n+1$ for certain isomorphic subgroups of $R\bar{3}$. Such values are actually being observed, e.g. $p = 31$ for $PtCl_3$ [3] as a hettotype of fcc packing. The necessary information for such relations is contained in Volume *A*1.

[1] *International Tables for Crystallography*, *Vol. A1*, 2004, Dordrecht: Kluwer. [2] Hoffmann R.-D., Pöttgen R., *Z. Kristallogr.* 2001, **216**, 127. [3] Müller U., *Z. Anorg. Allg. Chem.*, 2004, **630**, 1519.
Keywords: group-subgroup relations, subgroups,Wykoff positions

OCM07.27.6
Acta Cryst. (2005). A**61**, C132
Volume G: Definition and Exchange of Crystallographic Data
Sydney Hall[a], Brian McMahon[b], [a]*School of Biomedical and Chemical Sciences, University of Western Australia, Nedlands, Australia.* [b]*International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.* E-mail: syd.hall@bcs.uwa.edu.au

Volume G[1] will be launched at this congress. The highly data-dependent nature of crystallographic studies places great importance on the need for orderly acquisition and retention of data, and for computational tools that facilitate efficient data handling. To support this data-rich environment, Volume G is dedicated to the precise definition of the most commonly used data items. Although it focuses on the Crystallographic Information File (CIF) representation of data adopted by the IUCr in 1990 for journal submissions, it also considers more recent data-language developments involving XML.

CIF data dictionaries are described for *core*, *macromolecular*, *powder*, *symmetry*, *modulated-structure* and *precision-density* studies. The underpinning dictionary languages are also detailed, as are approaches for defining and storing image (binary) data. In these dictionaries, each data item is defined in terms of attributes that characterise their allowed values and mutual relationships. These provide human-readable and machine-readable descriptions of the data. However, the main use of the definitions is in a computer-software environment, so details of computer programs and libraries used with the electronic dictionaries to validate and exchange data items are also described. A CD-ROM will accompany the volume.

[1] International Tables for Crystallography, 2005, Volume G, *Definition and exchange of crystallographic data*, edited by S.R. Hall & B. McMahon, Heidelberg: Springer.
Keywords: International Tables, CIF dictionaries, data definition

OCM07.27.7
Acta Cryst. (2005). A**61**, C132
Status of Volume A: Space-group Symmetry
Theo Hahn, *Institut für Kristallographie, RWTH Aachen, Germany.* E-mail: hahn@xtal.rwth-aachen.de

Volume A treats space groups and their applications in all fields of crystallographic research and teaching. The subject matter is presented in three parts of different length and complexity:

(i) Central core of the volume are the plane-group and space-group tabulations in Parts 6 and 7 (620 pages, two pages per group).

(ii) The first 90 pages (Parts 1 to 5) contain definitions, guides to the tables and *practical* hints for the use of the space-group data on a level corresponding to an *elementary* textbook. These parts, as well as 24 selected space-group examples, also form the "*Brief Teaching Edition of Volume A*", which is intended as a brief, inexpensive tool for class-room teaching.

(iii) The final 180 pages of text (Parts 8 to 15) are of a much higher *theoretical* level and in some places correspond to an *advanced* text book of crystallographic symmetry.

The first edition of Volume A was published in 1983, of the Teaching Edition in 1985. The fifth revised editions of both volumes appeared in 2002. These editions are based completely on electronic files, both for tables and text (*c.f. Foreword to the Fifth Edition*). A corrected reprint of the fifth edition, as well as an on-line version, of Vol. A are in preparation and scheduled for 2005.

In order to honor two deceased authors of Volume A and their contributions, two special topics will be briefly discussed: (1) P. M. de Wolff (Delft): Reduced bases and lattice characters; (2) E. F. Bertaut (Grenoble): Extended Hermann-Mauguin space-group symbols and subgroups.
Keywords: space groups, symmetry, International Tables

OCM07.27.8
Acta Cryst. (2005). A**61**, C132
Status of Volume B: Reciprocal Space – planned 3rd Edition
Uri Shmueli, *School of Chemistry, Tel Aviv University, 69978 Tel Aviv, Israel.* E-mail: ushmueli@post.tau.ac.il

The second edition of Volume B was published in 2001 and its third edition is being planned. The subdivision of the volume in five parts remains unchanged but several changes are envisaged within most parts. Among the major revisions and additions are the following:

(i) Discussions of applications of direct methods to macromolecular crystallography will be greatly expanded; (ii) Patterson and molecular-replacement techniques will be revised, also in view of their appearance in Volume F; (iii) several major changes are expected to occur in the chapter on electron diffraction and microscopy in structure determination: a new Foreword, a thorough revision of the sections on convergent-beam electron diffraction and three-dimensional reconstruction and a new section on single-particle reconstruction; (iv) the chapter on molecular modeling and computer graphics will be enriched by a section on modern graphics software for structures consisting of small and medium-sized molecules; (v) a new chapter is being written on modern extensions of the Ewald method: (a) use of FFT in efficient computation of lattice sums, and (b) departures from the usual point-charge model; (vi) a significant revision is planned of the chapter on disorder diffuse scattering of X-rays and neutrons, and (vii) the chapter on reciprocal-space images of aperiodic crystals will be revised in view of recent developments.

Details on the second edition and the above plans can be found at:
http://www.iucr.org/iucr-top/it/itb/itb.html - IUCr office
http://crystal.tau.ac.il/xtal/comit/index.html - author's office
Keywords: International Tables, reciprocal space, methodology

OCM07.27.9
Acta Cryst. (2005). A**61**, C132-C133
Update on International Tables for Crystallography Volume F
Eddy Arnold[a], Michael G. Rossmann[b], [a]*Center for Advanced Biotechnology and Medicine, and Department of Chemistry and Chemical Biology, Rutgers University, Piscataway, NJ, USA.*